# Final Technical Report Contract NAS8-39131 Delivery Item # 3

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#### Contents:

I. Rutherford Backscattering Spectrometry (JRW) - N/A

II. Auger Electron Spectroscopy (MJB) - N/A

III. Ellipsometry (ATF)

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## I. INTRODUCTION

The multilayer Ellipsometry program has been developed with which the thickness and the optical properties of top layer can be determined with the additional information obtained from other measurement such as the optical constant of the middle layer film. Once the proper parameters are input into the program, the multilayer Ellipsometry program which was developed by H. Kim and Dr. Fromhold gives the best possible set of the solutions for the top layer thickness or its optical index graphically on a PC screen.

However at the time of measurement for the NASA samples with the latest multilayer Ellipsometry program developed in Auburn Ellipsometry Lab all the samples were called back so that we could not complete the measurement with the samples ellipsometrically.

In this report the basic two layer Ellipsometry theory will be summarized briefly as well as the one layer case. All the code is written in Microsoft Quickbasic version 4.5 for IBM PC with a VGA color graphics monitor so that the measurement could be cross-checked out graphically on the screen. The source code can be available from our Lab on the request.

## 2. ELLISOMETRY ONE LAYER THEORY

Ellipsometry is the measurement of the phase shift,  $\Delta$ , and the relative attenuation of the parallel and the perpendicular component of the electric vector to the plane of incidence,  $tan(\psi)$ . They contain the enough information to determine the thickness, the conductivity, or the index of optical constant. Measurement is so simple that it takes only several seconds with the Automated Ellipsometry system, but the proper theory and well implemented computer program must be utilized for the best result.

As indicated by Fig. 1, the electric vector of the reflected light is comprised of superimposed components due to multiple reflection within the dielectric film. Each reflection undergoes a phase retardation by

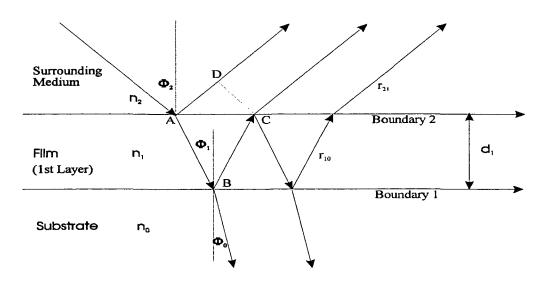


Figure 1

(1) 
$$\delta = k_1 \bullet (\overline{ABC}) - k_2 \bullet (\overline{CD}) = \left(\frac{4\pi \overline{n}_1 d_1}{\lambda_2}\right) \cos(\overline{\Phi}_1).$$

 $\lambda_2$  is the wavelength of the laser in the surrounding media in one layer film case; its value in air is 6328 A.

Application of this expression to multiple reflection theory enables us to write  $\Delta$  and  $\Psi$  in term of the phase shift  $\delta$ . Therefore we can calculate the thickness of the film, d, if the other parameters are known.

Two measurable quantities with ellipsometer  $\Psi$  and  $\Delta$  are defined as

(2) 
$$\tan \Psi e^{-i\Delta} = (E'_p / E'_s) / (E_p / E_s)$$
.

where

(3)  $\Delta$  = [Phase shift of the beam before and after reflection from the material surface]  $= (\beta_p - \beta_s)_{ref} - (\beta_p - \beta_s)_{inc}$ 

Primes on parameters indicate that those parameter values are for the reflected beam (i.e., after reflection from the sample surface); the non-primed parameters represent the corresponding quantities before reflection. (See Fig. 2).

## **Fresnel Coefficient**

If there exists a thin film (layer 1; see Fig. 1.) on the substrate, the total reflection from the thin film to the surrounding media, generally air, must be summed up the all of the multiple reflection and the multiple refraction between two boundaries (see Fig. 1.). In this case  $\Psi$  and  $\Delta$  are written explicitly;

$$(4) \qquad \tan\Psi \ e^{i\Delta} = \left(\frac{r_{21}^p + r_{10}^p \ e^{-i\delta}}{1 + \ r_{21}^p \ r_{10}^p e^{-i\delta}}\right) \left(\frac{1 + \ r_{21}^s \ r_{10}^s e^{-i\delta}}{r_{21}^s + r_{21}^s \ r_{10}^s \ e^{-i\delta}}\right),$$

where

(5) 
$$r_{10}^{p} = \frac{n_{0}\cos(\Phi_{1}) - n_{1}\cos(\Phi_{0})}{n_{0}\cos(\Phi_{1}) + n_{1}\cos(\Phi_{0})}$$

and

(6) 
$$r_{10}^{s} = \frac{n_1 \cos(\Phi_1) - n_0 \cos(\Phi_0)}{n_1 \cos(\Phi_1) + n_0 \cos(\Phi_0)}$$

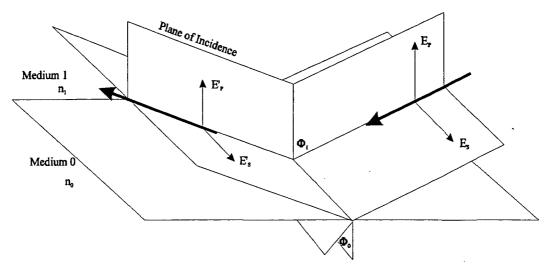


Figure 2

To measure the thickness of a film on a substrate, if the surrounding medium is air, Eq. (4) must be solved. This exact equation is so complicated that its solution cannot be readily obtained analytically. However if  $n_0$ ,  $n_1$ ,  $\lambda_2$  and  $\Phi_2$  are known, we can get the closest thickness to the actual thickness by using the complex quadratic formula. In Eq. (4), let  $\rho = \tan(\Psi) e^{-i\Delta}$  and  $Y = e^{-i\delta}$ , which leads to the quadratic equation

(7) 
$$EY^2 + BY + C = 0$$
,

where

(8) 
$$E = (\rho r_{21}^p r_{10}^p r_{10}^s) - (r_{21}^s r_{10}^s r_{10}^p)$$
,

(9) 
$$B = \rho (r_{21}^p r_{21}^s r_{10}^p + r_{10}^s) - (r_{21}^s r_{21}^p r_{10}^s + r_{10}^p) ,$$

(10) 
$$C = \rho r_{21}^s - r_{21}^p$$

and

(11) 
$$Y = e^{-i\delta}$$
.

At this point, Y can be obtained simply, and the thickness d can be calculated from Y,

(12) 
$$d = \delta \lambda_2 \cos(\overline{\phi}_1)/(4\pi \overline{n}_1)$$
.

If the film is absorbing, d is complex and we take only the real part of the thickness. The imaginary part depends on the experimental error. The smaller the imaginary part, the more accurate the thickness. Therefore if we measure the  $\Delta$  and  $\Psi$  with the ellipsometer, the thickness of a one-layer film can be calculated for either the nonobsorbing case or the absorbing case.

#### 3. ELLIPSOMETRY TWO LAYER THEORY

If a sample under measurement in air has two layers on a substrate, the format of the basic Ellipsometry equation still can be similar to Eq. (4) with minor change. The basic idea to deal with the two layer sample is to simplify the two layer model to one layer model by introducing a virtual substrate. The original substrate and the 1st layer can be considered as a substrate. Let R<sub>21</sub> the multiple reflection ratio from the boundary 2. Then the basic Ellipsometry equation can be written as

(13) 
$$\tan \Psi e^{i\Delta} = \left(\frac{r_{32}^p + R_{21}^p e^{-i\delta_2}}{1 + r_{32}^p R_{21}^p e^{-i\delta_2}}\right) \left(\frac{1 + r_{32}^s R_{21}^s e^{-i\delta_2}}{r_{32}^s + r_{32}^s R_{21}^s e^{-i\delta_2}}\right),$$

where

(14) 
$$R_{21}^p = \frac{r_{21}^p + r_{10}^p e^{-i\delta_1}}{1 + r_{21}^p r_{10}^p e^{-i\delta_1}}$$
,

(15) 
$$R_{21}^{s} = \frac{r_{21}^{s} + r_{10}^{s} e^{-i\delta_{1}}}{1 + r_{21}^{s} r_{10}^{s} e^{-i\delta_{1}}}$$
,

(16) 
$$r_{21}^p = \frac{n_1 \cos(\Phi_2) - n_2 \cos(\Phi_1)}{n_1 \cos(\Phi_2) + n_2 \cos(\Phi_1)}$$

and

(16) 
$$r_{21}^s = \frac{n_2 \cos(\Phi_2) - n_1 \cos(\Phi_1)}{n_2 \cos(\Phi_2) + n_1 \cos(\Phi_1)}$$
.

If d1, n0, n1, n2, n3 and  $\Phi$ 3 are known, Eq. (13) can be solved to obtain the thickness of top film as done in the section (2).

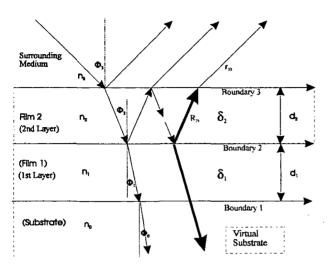


Figure 3

Let  $\rho=\tan(\Psi)$   $e^{i\Delta}$  and  $Y=e^{-i\delta_2}$  as we did in case of one layer model, then we have new quadratic equation

(17) 
$$EY^2 + BY + C = 0$$
,

where

(18) 
$$E = (\rho r_{32}^{p} R_{21}^{p} R_{21}^{s}) - (r_{32}^{s} R_{21}^{s} R_{21}^{p})$$

(19) 
$$B = \rho (r_{32}^p r_{32}^s R_{21}^p + R_{21}^s) - (r_{32}^s r_{32}^p R_{21}^s + R_{21}^p)$$
,

(20) 
$$C = \rho r_{32}^s - r_{32}^p$$
,

(21) 
$$r_{21}^{p} = \frac{n_{1}\cos(\Phi_{2}) - n_{2}\cos(\Phi_{1})}{n_{1}\cos(\Phi_{2}) + n_{2}\cos(\Phi_{1})} ,$$

and

(22) 
$$r_{21}^{s} = \frac{n_{2}\cos(\Phi_{2}) - n_{1}\cos(\Phi_{1})}{n_{2}\cos(\Phi_{2}) + n_{1}\cos(\Phi_{1})}$$
.

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